

Variations of Power-Expected-Posterior Priors in Normal Regression Models

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Abstract

The power-expected-posterior (PEP) prior is an objective prior for Gaussian linear models, which leads to consistent model selection inference and tends to favor parsimonious models. Recently, two new forms of the PEP prior were proposed which generalize its applicability to a wider range of models. We examine the properties of these two PEP variants within the context of the normal linear model, focusing on the prior dispersion and on the consistency of the induced model selection procedure. Results show that both PEP variants have larger variances than the unit-information g -prior and that they are consistent as the limiting behavior of the corresponding marginal likelihoods matches that of the BIC.

Keywords: expected-posterior prior, model selection consistency, linear regression, objective priors, power-expected-posterior prior; variable selection

1 Introduction

The power-expected-posterior (PEP) prior introduced by Fouskakis, Ntzoufras and Draper (2015) is an objective prior which amalgamates ideas from the power-prior (Ibrahim and Chen, 2000), the expected-posterior prior (Pérez and Berger, 2002) and Zellner’s (1986) g -prior. A central idea in the formulation of the PEP prior is the concept of “imaginary” data; specifically, for any given model $M_\ell \in \mathcal{M}$ with parameters of interest $\boldsymbol{\theta}_\ell$, the PEP prior can be defined as

$$\pi_\ell^{\text{PEP}}(\boldsymbol{\theta}_\ell, \boldsymbol{\psi}|\delta) = \pi_\ell^{\text{PEP}}(\boldsymbol{\theta}_\ell|\boldsymbol{\psi}, \delta)\pi^{\text{N}}(\boldsymbol{\psi}), \quad (1.1)$$

with

$$\pi_\ell^{\text{PEP}}(\boldsymbol{\theta}_\ell|\boldsymbol{\psi}, \delta) = \int \pi_\ell^{\text{N}}(\boldsymbol{\theta}_\ell|\mathbf{y}^*, \boldsymbol{\psi}, \delta)m_0^{\text{N}}(\mathbf{y}^*|\boldsymbol{\psi}, \delta)d\mathbf{y}^*, \quad (1.2)$$

where \mathcal{M} is the set of all models under consideration, $\boldsymbol{\psi}$ is a set of nuisance parameters common across all models $M \in \mathcal{M}$ and $\pi^{\text{N}}(\boldsymbol{\psi})$ is a prior distribution for $\boldsymbol{\psi}$. Under a

“baseline” prior $\pi_\ell^N(\boldsymbol{\theta}_\ell|\boldsymbol{\psi})$, the posterior distribution of $\boldsymbol{\theta}_\ell$ in (1.2) is conditioned upon the imaginary data $\mathbf{y}^* = (y_1^*, \dots, y_{n^*}^*)^T$, the nuisance parameters $\boldsymbol{\psi}$ and upon a parameter δ , which as explained next, regulates the spread of the distribution. This posterior distribution is averaged across the conditional predictive distribution $m_0^N(\mathbf{y}^*|\boldsymbol{\psi}, \delta)$ of a suitable reference model, say M_0 (with parameters $\boldsymbol{\theta}_0$ and $\boldsymbol{\psi}$), which is given by

$$m_0^N(\mathbf{y}^*|\boldsymbol{\psi}, \delta) = \int f_0(\mathbf{y}^*|\boldsymbol{\theta}_0, \boldsymbol{\psi}, \delta) \pi_0^N(\boldsymbol{\theta}_0|\boldsymbol{\psi}) d\boldsymbol{\theta}_0, \quad (1.3)$$

where $\pi_0^N(\boldsymbol{\theta}_0|\boldsymbol{\psi})$ is the “baseline” prior distribution for the parameters of model M_0 , before accounting for the imaginary data \mathbf{y}^* . The likelihood functions involved in the posterior distributions appearing in (1.2) and in (1.3) are defined as power functions of the original likelihoods, that is $f_\ell(\mathbf{y}^*|\boldsymbol{\theta}_\ell, \boldsymbol{\psi}, \delta) \propto f_\ell(\mathbf{y}^*|\boldsymbol{\theta}_\ell, \boldsymbol{\psi})^{1/\delta}$ for any $M_\ell \in \mathcal{M} \cup \{M_0\}$. Thus, the power parameter δ essentially regulates the contribution of the imaginary data on the PEP prior.

For a normal regression model M_ℓ , with coefficients $\boldsymbol{\beta}_\ell$ and error variance σ_ℓ^2 , Fouskakis et al. (2015) introduced the unconditional version of PEP by considering $\boldsymbol{\theta}_\ell = (\boldsymbol{\beta}_\ell, \sigma_\ell^2)$ and no nuisance parameters $\boldsymbol{\psi}$, while Fouskakis and Ntzoufras (2016) studied the conditional version of PEP with $\boldsymbol{\theta}_\ell = \boldsymbol{\beta}_\ell$ and common nuisance parameter across all models $\boldsymbol{\psi} = \sigma^2 = \sigma_\ell^2$, $\forall M_\ell \in \mathcal{M} \cup \{M_0\}$. In both of these settings it is natural to consider the density normalized power-likelihoods

$$f_\ell(\mathbf{y}^*|\boldsymbol{\beta}_\ell, \sigma^2, \delta, \mathbf{X}_\ell^*) = \frac{f_\ell(\mathbf{y}^*|\boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell^*)^{1/\delta}}{\int f_\ell(\mathbf{y}^*|\boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell^*)^{1/\delta} d\mathbf{y}^*}, \text{ for any } M_\ell \in \mathcal{M} \cup \{M_0\} \quad (1.4)$$

which are also normal distributions with variances inflated by a factor of δ . The default choice for δ is to set it equal to n^* , i.e. the sample size of the imaginary data, so that the overall information of the imaginary data in the posterior is equal to one data point. Furthermore, setting $n^* = n$ and, consequently, the design matrix of the imaginary data $\mathbf{X}_\ell^* \equiv \mathbf{X}_\ell$ simplifies significantly the overwhelming computations required when considering all possible “minimal” training samples (Pérez and Berger, 2002) while it also avoids the complicated issue (in some cases) of defining the size of the minimal training samples (Berger and Pericchi, 2004). In addition, under the choice $n^* = n$ the PEP prior remains relatively non-informative even for models with dimension close to the sample size n , while the effect on the evaluation of each model is minimal since the resulting Bayes factors are robust over different values of n^* . Detailed information about the default specifications of the PEP prior is provided in Fouskakis et al. (2015). Finally, the null model is a standard choice for the reference model in regression problems; see, for example, in Pérez and Berger (2002).

A limitation of the original PEP formulation is that the normalization of the power-likelihood, involved in the derivation of the prior, does not always lead to distributions of known form. Fouskakis, Ntzoufras and Perrakis (2016) tackled this problem by introducing two alternative definitions of the PEP prior suitable for more general model formulations and provided a computational solution for variable selection in generalized

linear models. However, the properties of these new versions of the PEP prior remain unexplored. In this paper, we study and compare their properties, by examining the dispersion of the conditional PEP variants and the consistency of the induced model selection procedures within the framework of the Gaussian linear model under the $\boldsymbol{\theta}_\ell = \boldsymbol{\beta}_\ell$, $\boldsymbol{\psi} = \sigma^2$ setting.

2 PEP prior variants

In what follows, we present two alternative definitions of the PEP prior in Gaussian regression models. We consider models M_ℓ with likelihood specified by

$$(\mathbf{Y}|\mathbf{X}_\ell, \boldsymbol{\beta}_\ell, \sigma^2, M_\ell) \sim N_n(\mathbf{X}_\ell \boldsymbol{\beta}_\ell, \sigma^2 \mathbf{I}_n), \quad (2.1)$$

where $\mathbf{Y} = (Y_1, \dots, Y_n)$ is a vector containing the (real-valued) responses for all subjects, \mathbf{X}_ℓ is an $n \times d_\ell$ design matrix containing the values of the explanatory variables in its columns, \mathbf{I}_n is the $n \times n$ identity matrix, $\boldsymbol{\beta}_\ell$ is a vector of length d_ℓ summarizing the effects of the covariates in model M_ℓ on the response \mathbf{Y} and σ^2 is the common error variance for all models M_ℓ .

The core idea in Fouskakis et al. (2016) is to use the unnormalized power likelihood $f_\ell(\mathbf{y}^*|\boldsymbol{\beta}_\ell, \sigma^2)^{1/\delta}$ and normalize the posterior density instead of the sampling distribution. This is also the approach followed by Ibrahim and Chen (2000) and Friel and Pettitt (2008, Eq.4). Specifically, the posterior distribution inside the integral of (1.2) is derived as

$$\pi_\ell^N(\boldsymbol{\beta}_\ell|\mathbf{y}^*, \sigma^2, \delta, \mathbf{X}_\ell^*) = \frac{f_\ell(\mathbf{y}^*|\boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell^*)^{1/\delta} \pi_\ell^N(\boldsymbol{\beta}_\ell|\sigma^2, \mathbf{X}_\ell^*)}{\int f_\ell(\mathbf{y}^*|\boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell^*)^{1/\delta} \pi_\ell^N(\boldsymbol{\beta}_\ell|\sigma^2, \mathbf{X}_\ell^*) d\boldsymbol{\beta}_\ell}. \quad (2.2)$$

Given this formulation, the two alternative PEP variants are defined as follows.

Definition 1 *The diffuse-reference PEP (DR-PEP) prior of model parameters $\boldsymbol{\beta}_\ell$ is defined as the power-posterior of $\boldsymbol{\beta}_\ell$ in (2.2) “averaged” over all imaginary data coming from the prior predictive distribution of the reference model M_0 based on the unnormalized likelihood, that is*

$$\begin{aligned} \pi_\ell^{\text{DR-PEP}}(\boldsymbol{\beta}_\ell|\sigma^2, \delta, \mathbf{X}_\ell^*) &= \mathbb{E}_{\mathbf{y}^*|\sigma^2, \delta, M_0, \mathbf{X}_0^*} \left[\pi_\ell^N(\boldsymbol{\beta}_\ell|\mathbf{y}^*, \sigma^2, \delta, \mathbf{X}_\ell^*) \right] \\ &= \int \pi_\ell^N(\boldsymbol{\beta}_\ell|\mathbf{y}^*, \sigma^2, \delta, \mathbf{X}_\ell^*) m_0^N(\mathbf{y}^*|\sigma^2, \delta, \mathbf{X}_0^*) d\mathbf{y}^* \\ \text{with } m_0^N(\mathbf{y}^*|\sigma^2, \delta, \mathbf{X}_0^*) &= \frac{\int f_0(\mathbf{y}^*|\beta_0, \sigma^2, \mathbf{X}_0^*)^{1/\delta} \pi_0^N(\beta_0|\sigma^2, \mathbf{X}_0^*) d\beta_0}{\int \int f_0(\mathbf{y}^*|\beta_0, \sigma^2, \mathbf{X}_0^*)^{1/\delta} \pi_0^N(\beta_0|\sigma^2, \mathbf{X}_0^*) d\beta_0 d\mathbf{y}^*}. \end{aligned}$$

Definition 2 *The concentrated-reference PEP (CR-PEP) prior of model parameters $\boldsymbol{\beta}_\ell$ is defined as the power-posterior of $\boldsymbol{\beta}_\ell$ in (2.2) “averaged” over all imaginary*

data coming from the prior predictive distribution of the reference model M_0 based on the actual likelihood, that is

$$\begin{aligned}\pi_\ell^{\text{CR-PEP}}(\boldsymbol{\beta}_\ell|\sigma^2, \delta, \mathbf{X}_\ell^*) &= \mathbb{E}_{\mathbf{y}^*|\sigma^2, M_0, \mathbf{X}_0^*} \left[\pi_\ell^{\text{N}}(\boldsymbol{\beta}_\ell|\mathbf{y}^*, \sigma^2, \delta, \mathbf{X}_\ell^*) \right] \\ &= \int \pi_\ell^{\text{N}}(\boldsymbol{\beta}_\ell|\mathbf{y}^*, \sigma^2, \delta, \mathbf{X}_\ell^*) m_0^{\text{N}}(\mathbf{y}^*|\sigma^2, \mathbf{X}_0^*) d\mathbf{y}^* \\ \text{with } m_0^{\text{N}}(\mathbf{y}^*|\sigma^2, \mathbf{X}_0^*) &= \int f_0(\mathbf{y}^*|\beta_0, \sigma^2, \mathbf{X}_0^*) \pi_0^{\text{N}}(\beta_0|\sigma^2, \mathbf{X}_0^*) d\beta_0.\end{aligned}$$

The above priors will be well defined under similar assumptions as in Pérez and Berger (2002). Furthermore, impropriety of the baseline priors does not cause indeterminacy to the resulting Bayes factors, since $\pi_\ell^{\text{CR-PEP}}(\boldsymbol{\beta}_\ell|\sigma^2, \delta, \mathbf{X}_\ell^*)$ depends only on the normalizing constant of the baseline prior of the parameter of the null model and in $\pi_\ell^{\text{DR-PEP}}(\boldsymbol{\beta}_\ell|\sigma^2, \delta, \mathbf{X}_\ell^*)$ the normalizing constants cancel out. For details see Fouskakis et al. (2016).

3 Properties of PEP variants in normal regression

In this section we examine the properties of the DR-PEP and CR-PEP priors and compare them to the corresponding properties of the original PEP prior. We work within the conjugate framework considered in Fouskakis and Ntzoufras (2016); specifically, we use as baseline priors a Zellner's g -prior for $\boldsymbol{\beta}_\ell$ conditional on σ^2 and a reference prior for σ^2 , that is

$$\pi_\ell^{\text{N}}(\boldsymbol{\beta}_\ell|\sigma^2, \mathbf{X}_\ell^*) = f_{N_{d_\ell}}(\boldsymbol{\beta}_\ell; \mathbf{0}, g_0(\mathbf{X}_\ell^{*T} \mathbf{X}_\ell^*)^{-1} \sigma^2) \text{ and } \pi^{\text{N}}(\sigma^2) \propto \sigma^{-2},$$

where d_ℓ is the dimension of $\boldsymbol{\beta}_\ell$ and $f_{N_k}(\cdot; \boldsymbol{\mu}, \boldsymbol{\Sigma})$ is the density function of the k -dimensional multivariate normal distribution with mean vector $\boldsymbol{\mu}$ and variance-covariance matrix $\boldsymbol{\Sigma}$. In the following we use the default values for the hyperparameters discussed in Section 1, namely $\delta = n$, $n^* = n$, $\mathbf{X}_\ell^* = \mathbf{X}_\ell$. In addition, following Fouskakis and Ntzoufras (2016) we set $g_0 = n^2$; this way, the overall contribution of the PEP prior to the posterior will be equal to $(1 + 1/n)$ data points, corresponding to one point contributed from the power-likelihood part and $1/n$ from the baseline g -prior. As reference model M_0 we consider the simplest nested model under consideration.

3.1 Power-posterior component in PEP variants

Under both Definitions 1 and 2 and for any given model M_ℓ , the unnormalized likelihood is given by

$$\begin{aligned}f_\ell(\mathbf{y}^* | \boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell) &^{1/\delta} = f_{N_n}(\mathbf{y}^*; \mathbf{X}_\ell \boldsymbol{\beta}_\ell, \sigma^2 \mathbf{I}_n)^{1/\delta} \\ &= (2\pi\sigma^2\delta)^{\frac{n}{2}} (2\pi\sigma^2)^{-\frac{n}{2\delta}} \times \\ &\quad \times \left[(2\pi\sigma^2\delta)^{-\frac{n}{2}} \exp \left(-\frac{1}{2\sigma^2\delta} (\mathbf{y}^* - \mathbf{X}_\ell \boldsymbol{\beta}_\ell)^T (\mathbf{y}^* - \mathbf{X}_\ell \boldsymbol{\beta}_\ell) \right) \right] \\ &= \delta^{\frac{n}{2}} (2\pi\sigma^2)^{\frac{n(\delta-1)}{2\delta}} f_{N_n}(\mathbf{y}^*; \mathbf{X}_\ell \boldsymbol{\beta}_\ell, \sigma^2 \delta \mathbf{I}_n).\end{aligned}\tag{3.1}$$

Therefore, for both DR-PEP and CR-PEP priors, the posterior distribution (2.2), conditional on the imaginary data, is given by

$$\begin{aligned}
\pi_\ell^N(\boldsymbol{\beta}_\ell | \mathbf{y}^*, \sigma^2, \delta, \mathbf{X}_\ell) &\propto f_\ell(\mathbf{y}^* | \boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell)^{1/\delta} \pi_\ell^N(\boldsymbol{\beta}_\ell | \sigma^2, \mathbf{X}_\ell), \\
&\propto f_{N_n}(\mathbf{y}^*; \mathbf{X}_\ell \boldsymbol{\beta}_\ell, \mathbf{I}_n \delta \sigma^2) f_{N_{d_\ell}}(\boldsymbol{\beta}_\ell; \mathbf{0}, g_0(\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \sigma^2) \\
&= f_{N_{d_\ell}}(\boldsymbol{\beta}_\ell; w \hat{\boldsymbol{\beta}}_\ell^*, w \delta (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \sigma^2),
\end{aligned} \tag{3.2}$$

where $w = g_0/(g_0 + \delta)$ and $\hat{\boldsymbol{\beta}}_\ell^*$ is the maximum likelihood estimate based on the imaginary response \mathbf{y}^* . Thus, the posterior distribution involved in the Definitions 1 and 2 is identical to the corresponding posterior under the original conditional PEP prior; see Equation 3 in Fouskakis and Ntzoufras (2016).

3.2 Prior distributions and dispersion

3.2.1 Diffuse-reference PEP prior

For the DR-PEP setup, the prior predictive distribution of the imaginary data under model M_ℓ is given by

$$m_\ell^N(\mathbf{y}^* | \sigma^2, \delta, \mathbf{X}_\ell) = \frac{m_\ell^U(\mathbf{y}^* | \sigma^2, \delta, \mathbf{X}_\ell)}{\int m_\ell^U(\mathbf{y}^* | \sigma^2, \delta, \mathbf{X}_\ell) d\mathbf{y}^*},$$

where $m_\ell^U(\mathbf{y}^* | \sigma^2, \delta, \mathbf{X}_\ell)$ is the normalizing constant of the power-posterior in (2.2) which is derived as follows

$$\begin{aligned}
m_\ell^U(\mathbf{y}^* | \sigma^2, \delta, \mathbf{X}_\ell) &= \int f_\ell(\mathbf{y}^* | \boldsymbol{\beta}_\ell, \sigma^2, \mathbf{X}_\ell)^{1/\delta} \pi_\ell^N(\boldsymbol{\beta}_\ell | \sigma^2, \mathbf{X}_\ell) d\boldsymbol{\beta}_\ell \\
&= \delta^{\frac{n}{2}} (2\pi\sigma^2)^{\frac{n(\delta-1)}{2\delta}} \times \\
&\quad \times \int f_{N_n}(\mathbf{y}^*; \mathbf{X}_\ell \boldsymbol{\beta}_\ell, \sigma^2 \delta \mathbf{I}_n) f_{N_{d_\ell}}(\boldsymbol{\beta}_\ell; \mathbf{0}, g_0(\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \sigma^2) d\boldsymbol{\beta}_\ell \\
&= \delta^{\frac{n}{2}} (2\pi\sigma^2)^{\frac{n(\delta-1)}{2\delta}} f_{N_n}(\mathbf{y}^*; \mathbf{0}, \boldsymbol{\Lambda}_\ell^{-1} \sigma^2),
\end{aligned} \tag{3.3}$$

with

$$\boldsymbol{\Lambda}_\ell^{-1} = \delta \mathbf{I}_n + g_0 \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T \text{ and } \boldsymbol{\Lambda}_\ell = \delta^{-1} (\mathbf{I}_n - w \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T).$$

From the previous equations, it immediately follows that

$$m_0^N(\mathbf{y}^* | \sigma^2, \delta, \mathbf{X}_0) = f_{N_n}(\mathbf{y}^*; \mathbf{0}, \boldsymbol{\Lambda}_0^{-1} \sigma^2) \tag{3.4}$$

with

$$\boldsymbol{\Lambda}_0^{-1} = \delta \mathbf{I}_n + \frac{g_0}{n} \mathbf{1}_n \mathbf{1}_n^T \text{ and } \boldsymbol{\Lambda}_0 = \delta^{-1} (\mathbf{I}_n - \frac{w}{n} \mathbf{1}_n \mathbf{1}_n^T). \tag{3.5}$$

Thus, both components of the DR-PEP prior, that is the power-posterior in (3.2) and the prior predictive in (3.4), are exactly the same as the corresponding components

of the conditional PEP approach of Fouskakis and Ntzoufras (2016), where the density-normalized likelihood in (1.4) was used. Hence, for Gaussian linear models the DR-PEP prior coincides to the original version of the conditional PEP and is given by

$$\begin{aligned}\pi_{\ell}^{\text{DR-PEP}}(\boldsymbol{\beta}_{\ell} | \sigma^2, \delta, \mathbf{X}_{\ell}) &= f_{N_{d_{\ell}}}(\boldsymbol{\beta}_{\ell}; \mathbf{0}, \mathbf{V}_{\ell} \sigma^2), \\ \mathbf{V}_{\ell} &= \delta (\mathbf{X}_{\ell}^T [w^{-1} \mathbf{I}_n - (\delta \boldsymbol{\Lambda}_0 + w \mathbf{H}_{\ell})^{-1}] \mathbf{X}_{\ell})^{-1}\end{aligned}\quad (3.6)$$

with $\mathbf{H}_{\ell} = \mathbf{X}_{\ell}(\mathbf{X}_{\ell}^T \mathbf{X}_{\ell})^{-1} \mathbf{X}_{\ell}^T$ and $\boldsymbol{\Lambda}_0$ given in (3.5).

The volume of dispersion of the DR-PEP prior is given by the determinant of the covariance matrix \mathbf{V}_{ℓ} and equals

$$|\mathbf{V}_{\ell}| = \xi \times |\mathbf{X}_{\ell}^T \mathbf{X}_{\ell}|^{-1} \text{ with } \xi = \{\delta w(w+1)\}^{d_{\ell}-d_0} g^{d_0}. \quad (3.7)$$

For the default values $\delta = n$ and $g_0 = n^2$, the variance multiplier ξ appearing in (3.7) is equal to

$$\xi = n^{2d_{\ell}} \left[\frac{2n+1}{(n+1)^2} \right]^{d_{\ell}-d_0} > n^{d_{\ell}}, \quad (3.8)$$

where on the right hand side of the inequality we have the corresponding variance multiplier of Zellner's unit-information g -prior. The result in (3.8) holds since

$$\begin{aligned}\phi(n) &= \log \xi - d_{\ell} \log n \\ &= d_{\ell} \log n + (d_{\ell} - d_0) \log \left[\frac{2n+1}{(n+1)^2} \right]\end{aligned}\quad (3.9)$$

is an increasing function of n and $\phi(2) > 0$; see Fouskakis and Ntzoufras (2016) for details. Hence, the DR-PEP prior is more dispersed than Zellner's g -prior with $g = n$, for any sample size $n \geq 2$, and consequently it leads to a more parsimonious variable selection procedure.

3.2.2 Concentrated-reference PEP prior

Under the CR-PEP approach, the prior predictive of the imaginary data is given by

$$m_0^N(\mathbf{y}^* | \sigma^2, \mathbf{X}_0) = f_{N_n}(\mathbf{y}^*; \mathbf{0}, [\boldsymbol{\Lambda}_0^{(\text{CR})}]^{-1} \sigma^2), \quad (3.10)$$

with

$$[\boldsymbol{\Lambda}_0^{(\text{CR})}]^{-1} = \mathbf{I}_n + g_0 n^{-1} \mathbf{1}_n \mathbf{1}_n^T \text{ and } \boldsymbol{\Lambda}_0^{(\text{CR})} = \mathbf{I}_n - \frac{g_0}{g_0 + 1} n^{-1} \mathbf{1}_n \mathbf{1}_n^T.$$

Combining (3.2) and (3.10), we obtain the CR-PEP prior which has the same form as the DR-PEP in (3.6) but with variance-covariance matrix

$$\mathbf{V}_{\ell}^{(\text{CR})} = \delta (\mathbf{X}_{\ell}^T [w^{-1} \mathbf{I}_n - (\delta \boldsymbol{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_{\ell})^{-1}] \mathbf{X}_{\ell})^{-1}.$$

As seen, the CR-PEP and DR-PEP priors differ only with respect to the variance-covariance matrix \mathbf{V}_ℓ appearing in (3.6) where $\mathbf{\Lambda}_0$ is substituted by $\mathbf{\Lambda}_0^{(\text{CR})}$. The volume of dispersion is now given by

$$|\mathbf{V}_\ell^{(\text{CR})}| = \xi \times |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} \text{ with } \xi = w^{d_\ell} (w + \delta)^{d_\ell - d_0} (w + \delta + w g_0)^{d_0}. \quad (3.11)$$

For the derivation of the result in (3.11) see Appendix A. Under the default setting $\delta = n$ and $g_0 = n^2$, the variance multiplier becomes

$$\xi = n^{2d_\ell} \left[\frac{n+2}{(n+1)^2} \right]^{d_\ell} \left[\frac{n^2+n+2}{n+2} \right]^{d_0}. \quad (3.12)$$

The log-ratio of the variance multipliers of the CR-PEP prior and the unit-information g -prior is given by

$$\begin{aligned} \phi(n) &= \log \xi - d_\ell \log n \\ &= d_\ell \log \left(\frac{n^2 + 2n}{n^2 + 2n + 1} \right) + d_0 \log \left(\frac{n^2 + n + 2}{n + 2} \right). \end{aligned} \quad (3.13)$$

The first derivative of the function in (3.13) is positive, but in this case $\phi(n)$ is not positive for any value of n , d_ℓ and d_0 . However, throughout this paper, we consider the case where M_0 is nested to M_ℓ . Moreover it is realistic to require that the sample size needs to be at least equal to $d_\ell + 1$ (in order to be able to estimate all model parameters). Hence, we can safely work under the restriction $1 \leq d_0 < d_\ell \leq n - 1$. Notice that the left and right terms in (3.13) are strictly negative and positive, respectively; therefore, substituting d_ℓ by its upper bound (equal to $n - 1$) and d_0 by its lower bound (equal to one) we obtain

$$\begin{aligned} d_\ell \log \left(\frac{n^2 + 2n}{n^2 + 2n + 1} \right) + d_0 \log \left(\frac{n^2 + n + 2}{n + 2} \right) &\geq \\ (n - 1) \log \left(\frac{n^2 + 2n}{n^2 + 2n + 1} \right) + \log \left(\frac{n^2 + n + 2}{n + 2} \right) &= \phi^*(n), \end{aligned} \quad (3.14)$$

for $d_0 \in [1, n - 2]$, $d_\ell \in [d_0 + 1, n - 1]$ and any $n \in \mathbb{Z}^+$. Plotting $\phi^*(n)$ in (3.14) reveals that this function is always positive; therefore, the log-ratio of the variance multipliers in (3.13) will also be positive under the working constraints. Thus, the variance of the CR-PEP prior is larger than that of the g -prior, which means that CR-PEP prior will in general tend to favour less complex models. Additionally, by rewriting the variance multiplier in (3.12) as

$$\xi = n^{d_\ell} \left[\frac{n^2 + 2n}{n^2 + 2n + 1} \right]^{d_\ell} \left[\frac{n^2 + n + 2}{n + 2} \right]^{d_0}, \quad (3.15)$$

we can see that for relatively large n the first fraction in (3.15) tends to one while the second fraction tends to n . Assuming that $d_0 = 1$, the CR-PEP variance multiplier is then approximately equal to $n^{d_\ell+1}$ and the log-ratio in (3.13) will be $\phi(n) \approx \log(n^{d_\ell+1}/n^{d_\ell}) =$

$\log(n)$. When the reference model M_0 is not the null model, the corresponding approximation is equal to $d_0 \log(n)$.

The comparison with respect to the DR-PEP prior, and consequently to the original conditional PEP approach, is more straightforward. In this case, the log-ratio of the CR-PEP variance multiplier (3.15) over the corresponding multiplier of the DR-PEP prior, given in (3.8), is

$$\begin{aligned}
\varphi(n) &= \log \left(\left[\frac{n+2}{(n+1)^2} \right]^{d_\ell} \left[\frac{n^2+n+2}{n+2} \right]^{d_0} \left[\frac{2n+1}{(n+1)^2} \right]^{d_0-d_\ell} \right) \\
&= \log \left([n+2]^{d_\ell-d_0} [2n+1]^{d_0-d_\ell} \left[\frac{n^2+n+2}{(n+1)^2} \right]^{d_0} \right) \\
&= \log \left(\left[\frac{n+2}{2n+1} \right]^{d_\ell-d_0} \left[\frac{n^2+n+2}{n^2+2n+1} \right]^{d_0} \right). \tag{3.16}
\end{aligned}$$

Both fractions appearing in (3.16) are equal to or smaller than one for any $n \geq 1$. Therefore, the log-ratio is always negative. This implies that the CR-PEP prior induces a variable selection procedure which is less parsimonious than the corresponding one under the DR-PEP prior.

3.2.3 Numerical illustrations

Here we provide some basic illustrations that highlight the behavior of the variance multipliers of the CR-PEP and DR-PEP priors for varying sample size and number of predictors, given the restriction that $n \geq d_\ell + 1$ and assuming that $d_0 = 1$.

The log-ratios of the DR-PEP and CR-PEP prior multipliers over the unit-information g -prior multiplier (see respective Eqs. 3.9 and 3.13), for increasing sample size n and selected values of $d_\ell \in \{5, 10, 50, 100\}$, are illustrated in Figure 1. For both prior setups, the log-ratios are positive and increasing with the sample size n , with the DR-PEP being always more dispersed than the CR-PEP as expected according to Section 3.2.2. Additionally, the log-ratio of the DR-PEP prior over the g -prior increases as d_ℓ gets larger, whereas the ratio of the CR-PEP prior over the g -prior is not affected by d_ℓ as it remains constant, approximately equal to $\log(n)$.

In Figure 2 we present on log-scale the variance multipliers of the CR-PEP, DR-PEP and the unit-information g priors for $d_\ell \in \{10, 25, 50, 100\}$ and sample size ranging from 101 (the minimum size required for $d_\ell = 100$) to 1000. As seen, as model dimensionality increases all priors become more dispersed; however, the distance between the variance multiplier of the DR-PEP prior and the corresponding multipliers of the CR-PEP and the g -prior is also increasing with d_ℓ . Potentially, this feature of the DR-PEP prior makes it more suitable for problems involving a large number of predictors and where the aim is to have a parsimonious model selection method.

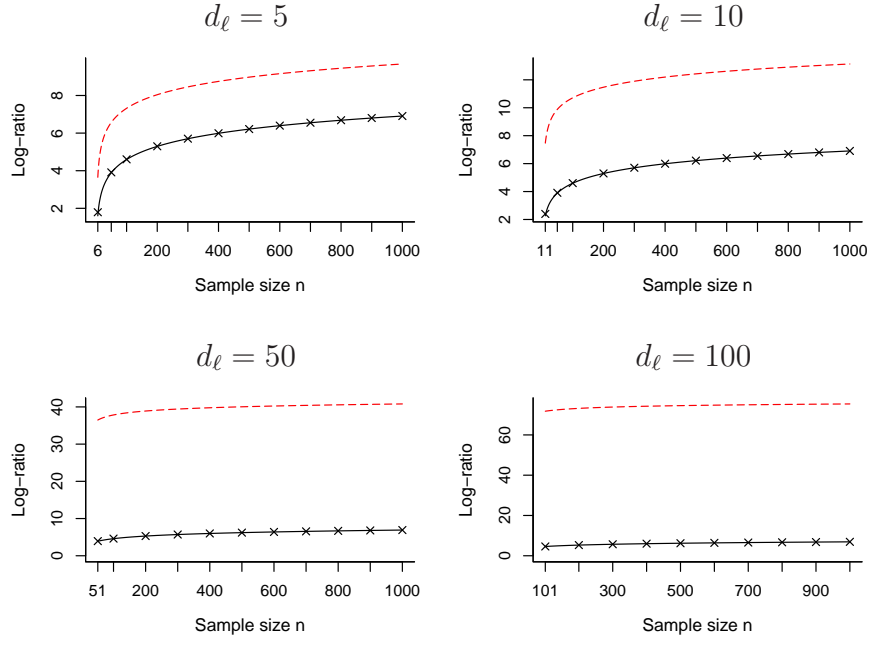


Figure 1: Log-ratios of the variance multipliers of the DR-PEP prior (dashed red line) and CR-PEP prior (solid black line) over the unit-information g -prior for $d_\ell = 5, 10, 50, 100$ and varying sample size; the crosses correspond to the approximation $\log(n)$.

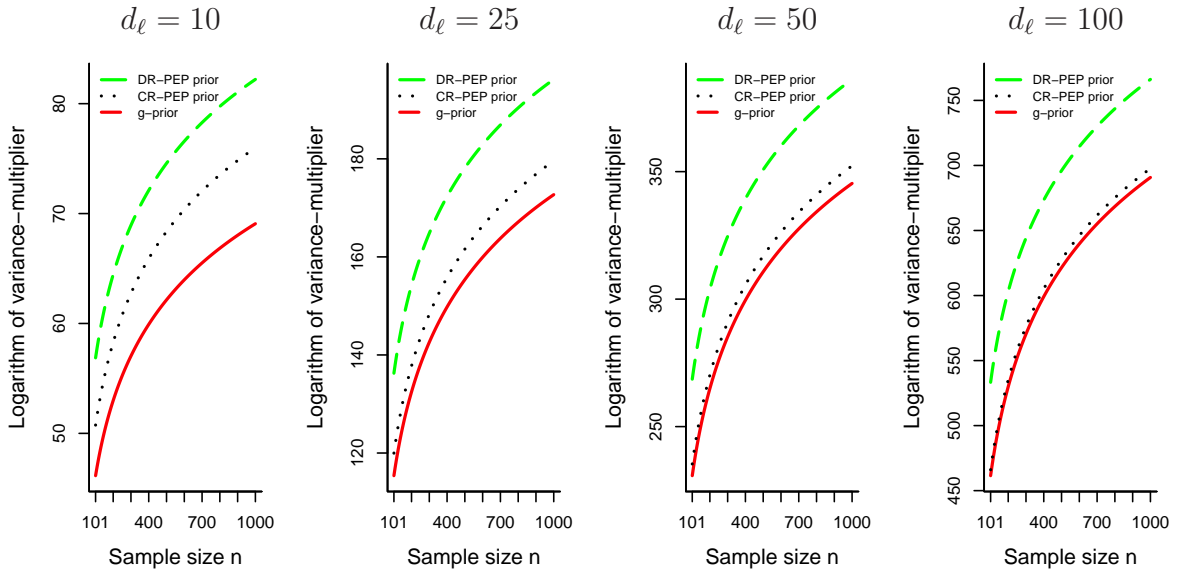


Figure 2: Log-scaled plots of the variance multipliers of the DR-PEP, CR-PEP and g priors for $d_\ell = 10, 25, 50, 100$ and sample size ranging from 101 to 1000.

3.3 Marginal likelihood and model selection consistency

The posterior distribution of β_ℓ and σ^2 under either the conditional PEP prior of Fouskakis and Ntzoufras (2016) or the DR-PEP prior, examined here, is given by

$$\pi_\ell^{\text{DR-PEP}}(\beta_\ell, \sigma^2 | \mathbf{y}, \delta, \mathbf{X}_\ell) = f_{N_{d_\ell}}(\beta_\ell; \tilde{\beta}_\ell, \tilde{\Sigma}_\ell \sigma^2) f_{IG}(\sigma^2; \tilde{a}_\ell, \tilde{b}_\ell), \quad (3.17)$$

where $\tilde{\beta}_\ell = \tilde{\Sigma}_\ell \mathbf{X}_\ell^T \mathbf{y}$, $\tilde{\Sigma}_\ell = (\mathbf{V}_\ell^{-1} + \mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1}$, $\tilde{a}_\ell = n/2$, $\tilde{b}_\ell = \text{SS}_\ell/2$ with $\text{SS}_\ell = \mathbf{y}^T (\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell \mathbf{X}_\ell^T)^{-1} \mathbf{y}$, and $f_{IG}(\cdot; a, b)$ denotes the density of the inverse gamma distribution with shape parameter a and scale parameter b . In the above, \mathbf{V}_ℓ is given in Section 3.2.1.

Then, the marginal log-likelihood is given by

$$\begin{aligned} \log m_\ell^{\text{DR-PEP}}(\mathbf{y} | \delta, \mathbf{X}_\ell) &= C - \frac{1}{2} \log |\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell \mathbf{X}_\ell^T| - \\ &\quad \frac{n}{2} \log (\mathbf{y}^T (\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell \mathbf{X}_\ell^T)^{-1} \mathbf{y}), \end{aligned} \quad (3.18)$$

where C is a constant that does not depend on the structure of model M_ℓ . For large n , the marginal log-likelihood in (3.18) can be approximated by

$$\log m_\ell^{\text{DR-PEP}}(\mathbf{y} | \delta, \mathbf{X}_\ell) \approx C - \frac{1}{2} \text{BIC}_\ell. \quad (3.19)$$

Thus, the marginal likelihood under the DR-PEP prior has the same limiting behavior as the BIC which is known to be consistent under a minor realistic assumption (Fernández, Ley and Steel, 2001, Liang, Paulo, Molina, Clyde and Berger, 2008). For a detailed proof of (3.19) see Fouskakis and Ntzoufras (2016).

Similarly to (3.18), the marginal log-likelihood under the CR-PEP prior is

$$\begin{aligned} \log m_\ell^{\text{CR-PEP}}(\mathbf{y} | \delta, \mathbf{X}_\ell) &= C - \frac{1}{2} \log |\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell^{(\text{CR})} \mathbf{X}_\ell^T| - \\ &\quad \frac{n}{2} \log (\mathbf{y}^T (\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell^{(\text{CR})} \mathbf{X}_\ell^T)^{-1} \mathbf{y}). \end{aligned} \quad (3.20)$$

Following the proof Fouskakis and Ntzoufras (2016, see Section D, Eqs. D.1–D.2 of the Supplementary Material), the first logarithmic term yields

$$\begin{aligned} |\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell^{(\text{CR})} \mathbf{X}_\ell^T| &= (1 + \delta w)^{d_\ell} |\mathbf{\Lambda}_0^{(\text{CR})}|^{-1} \left| \mathbf{\Lambda}_0^{(\text{CR})} + \left(\frac{w^2}{1 + \delta w} \right) \mathbf{H}_\ell \right| \\ &\approx (1 + \delta)^{d_\ell} |\mathbf{\Lambda}_0^{(\text{CR})}|^{-1} \left| \mathbf{\Lambda}_0^{(\text{CR})} + \left(\frac{1}{1 + \delta} \right) \mathbf{H}_\ell \right| \\ &\approx (1 + \delta)^{d_\ell}. \end{aligned} \quad (3.21)$$

Note that the approximation is accurate for large n when $\delta = n$ and $g_0 = n^2$, so that $w = g_0/(g_0 + \delta) \approx 1$. Given these values, we can also approximate the second logarithmic term in (3.20) by

$$\mathbf{y}^T (\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell^{(\text{CR})} \mathbf{X}_\ell^T)^{-1} \mathbf{y} \approx \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T \mathbf{y} \equiv \text{RSS}_\ell, \quad (3.22)$$

where RSS_ℓ is the usual residual sum of squares of model M_ℓ . The derivation for (3.22) is provided in Appendix B. Hence, the marginal log-likelihood under the CR-PEP prior is approximately given by

$$\begin{aligned}\log m_\ell^{\text{CR-PEP}}(\mathbf{y}|\delta, \mathbf{X}_\ell) &\approx C - \frac{d_\ell}{2} \log(n+1) - \frac{n}{2} \log(\text{RSS}_\ell) \\ &\approx C - \frac{d_\ell}{2} \log(n) - \frac{n}{2} \log(\text{RSS}_\ell) \\ &\approx C - \frac{1}{2} \text{BIC}_\ell,\end{aligned}\tag{3.23}$$

for $\delta = n$ and large n . Thus, variable selection, based on the CR-PEP prior with a g -prior as baseline, has also the same limiting behavior as the BIC and is, therefore, consistent.

4 Epilogue

In this paper we examined the properties of two new versions of the PEP prior, which have been recently proposed in the context of objective Bayes variable selection (Fouskakis et al., 2016), namely the CR-PEP and DR-PEP priors. Specifically, we compared the dispersion of these priors and investigated the aspect of model selection consistency under each prior in the normal linear regression model.

The main findings can be summarized as follows. In the Gaussian case, the DR-PEP prior coincides with the original conditional PEP prior of Fouskakis and Ntzoufras (2016), thus, sharing the same consistency and parsimony properties. On the other hand, the predictive distribution of the imaginary data used in the CR-PEP set-up, results in a PEP prior form which is less dispersed and, therefore, also less parsimonious than the DR-PEP prior. Nevertheless, the CR-PEP prior also leads to a consistent variable selection procedure. In addition, both priors have larger variances than the unit-information g -prior, which implies that they will support more parsimonious models than the g -prior. The DR-PEP prior in particular seems to be more suitable for large- p problems, as its variance ratio over the g -prior increases as the number of predictor variables becomes larger.

The results presented here concern the case of the Gaussian linear model, offering useful insights about the behavior of the DR/CR-PEP priors. The properties of these priors in generalized linear models is a topic that will be addressed in future work.

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Appendix

A Derivation of Equation 3.11

The determinant of the CR-PEP prior covariance matrix is

$$|\mathbf{V}_\ell^{(\text{CR})}| = \delta^{d_\ell} |w^{-1} \mathbf{X}_\ell^T \mathbf{X}_\ell - \mathbf{X}_\ell^T (\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell)^{-1} \mathbf{X}_\ell|^{-1}. \quad (\text{A.1})$$

Based on the matrix determinant Lemma (Harville, 1997, p.416), which states that $|\mathbf{A} + \mathbf{CBD}^T| = |\mathbf{A}| |\mathbf{B}| |\mathbf{B}^{-1} + \mathbf{D}^T \mathbf{A}^{-1} \mathbf{C}|$ for any square invertible matrices \mathbf{A} and \mathbf{B} , we can write (A.1) as

$$\begin{aligned} |\mathbf{V}_\ell^{(\text{CR})}| &= \delta^{d_\ell} \left(|w^{-1} \mathbf{X}_\ell^T \mathbf{X}_\ell| | - (\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell)^{-1} \times \right. \\ &\quad \left. \times | - (\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell) + w \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell) \mathbf{X}_\ell^T | \right)^{-1} \\ &= \delta^{d_\ell} w^{d_\ell} |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} |\delta \mathbf{\Lambda}_0^{(\text{CR})}|^{-1} |(\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell)|. \end{aligned} \quad (\text{A.2})$$

Using repeatedly the matrix determinant Lemma on the last term of (A.2) yields

$$\begin{aligned} |\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell| &= |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} \left| \mathbf{X}_\ell^T \mathbf{X}_\ell + \frac{w}{\delta} \mathbf{X}_\ell^T [\mathbf{\Lambda}_0^{(\text{CR})}]^{-1} \mathbf{X}_\ell \right| \\ &= |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} \left| \mathbf{X}_\ell^T \mathbf{X}_\ell + \frac{w}{\delta} \mathbf{X}_\ell^T (\mathbf{I}_n + g_0 \mathbf{X}_0 (\mathbf{X}_0^T \mathbf{X}_0)^{-1} \mathbf{X}_0^T) \mathbf{X}_\ell \right| \\ &= |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} \left| \mathbf{X}_\ell^T \mathbf{X}_\ell + \frac{w}{\delta} \mathbf{X}_\ell^T \mathbf{X}_\ell + \frac{w g_0}{\delta} \mathbf{X}_\ell^T \mathbf{X}_0 (\mathbf{X}_0^T \mathbf{X}_0)^{-1} \mathbf{X}_0^T \mathbf{X}_\ell \right| \\ &= |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} \left| \frac{w + \delta}{\delta} \mathbf{X}_\ell^T \mathbf{X}_\ell + \frac{w g_0}{\delta} \mathbf{X}_\ell^T \mathbf{X}_0 (\mathbf{X}_0^T \mathbf{X}_0)^{-1} \mathbf{X}_0^T \mathbf{X}_\ell \right| \\ &= |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1} \left(\frac{w + \delta}{\delta} \right)^{d_\ell} |\mathbf{X}_\ell^T \mathbf{X}_\ell| |\mathbf{X}_0^T \mathbf{X}_0|^{-1} \times \\ &\quad \times \left| \mathbf{X}_0^T \mathbf{X}_0 + \frac{w g_0}{\delta} \mathbf{X}_0^T \mathbf{X}_\ell \left(\frac{w + \delta}{\delta} \mathbf{X}_\ell^T \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{X}_0 \right| \\ &= \left(\frac{w + \delta}{\delta} \right)^{d_\ell} |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_0^T \mathbf{X}_0|^{-1} \times \\ &\quad \times \left| \mathbf{X}_0^T \mathbf{X}_0 + \frac{w g_0}{w + \delta} \mathbf{X}_0^T \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T \mathbf{X}_0 \right| \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} &= \left(\frac{w + \delta}{\delta} \right)^{d_\ell} |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_0^T \mathbf{X}_0|^{-1} \left| \mathbf{X}_0^T \mathbf{X}_0 + \frac{w g_0}{w + \delta} \mathbf{X}_0^T \mathbf{X}_0 \right| \\ &= \left(\frac{w + \delta}{\delta} \right)^{d_\ell} |\delta \mathbf{\Lambda}_0^{(\text{CR})}| |\mathbf{X}_0^T \mathbf{X}_0|^{-1} \left(\frac{w + \delta + w g_0}{w + \delta} \right)^{d_0} |\mathbf{X}_0^T \mathbf{X}_0| \\ &= (w + \delta)^{d_\ell - d_0} \delta^{-d_\ell} (w + \delta + w g_0)^{d_0} |\delta \mathbf{\Lambda}_0^{(\text{CR})}| \end{aligned} \quad (\text{A.4})$$

Note that the transition from (A.3) to the following equation is due to the fact that $\mathbf{X}_0^T \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T \mathbf{X}_0 = \mathbf{X}_0^T \mathbf{H}_\ell \mathbf{X}_0 = \mathbf{X}_0^T \mathbf{X}_0$, since $\mathbf{X}_0^T \mathbf{H}_\ell = \mathbf{X}_0^T$ for any sub-matrix \mathbf{X}_0 of \mathbf{X}_ℓ . From (A.2) and (A.4) we have that

$$|\mathbf{V}_\ell^{(\text{CR})}| = w^{d_\ell} (w + \delta)^{d_\ell - d_0} (w + \delta + w g_0)^{d_0} |\mathbf{X}_\ell^T \mathbf{X}_\ell|^{-1}. \quad (\text{A.5})$$

B Derivation of Equation 3.22

$$\begin{aligned} & \mathbf{y}^T (\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell^{(\text{CR})} \mathbf{X}_\ell^T)^{-1} \mathbf{y} \\ &= \mathbf{y}^T \left(\mathbf{I}_n - \mathbf{X}_\ell (\mathbf{V}_\ell^{(\text{CR})})^{-1} + \mathbf{X}_\ell^T \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y} \\ &= \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}_\ell \left(\delta^{-1} \left[\mathbf{X}_\ell^T \left(w^{-1} \mathbf{I}_n - (\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell)^{-1} \right) \mathbf{X}_\ell \right] + \mathbf{X}_\ell^T \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y} \\ &= \mathbf{y}^T \mathbf{y} - \delta \mathbf{y}^T \mathbf{X}_\ell \left(w^{-1} \mathbf{X}_\ell^T \mathbf{X}_\ell - \mathbf{X}_\ell^T (\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell)^{-1} \mathbf{X}_\ell + \delta \mathbf{X}_\ell^T \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y} \\ &= \mathbf{y}^T \mathbf{y} - \delta \mathbf{y}^T \mathbf{X}_\ell \left(\frac{1 + \delta w}{w} \mathbf{X}_\ell^T \mathbf{X}_\ell - \mathbf{X}_\ell^T (\delta \mathbf{\Lambda}_0^{(\text{CR})} + w \mathbf{H}_\ell)^{-1} \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y} \\ &= \mathbf{y}^T \mathbf{y} - \delta \mathbf{y}^T \mathbf{X}_\ell \left(\frac{1 + \delta w}{w} \mathbf{X}_\ell^T \mathbf{X}_\ell - \mathbf{X}_\ell^T \left(\delta \left(\mathbf{I}_n - \frac{g_0}{g_0 + 1} \mathbf{H}_0 \right) + w \mathbf{H}_\ell \right)^{-1} \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y} \\ &= \mathbf{y}^T \mathbf{y} - \frac{w \delta}{1 + w \delta} \mathbf{y}^T \mathbf{X}_\ell \left(\mathbf{X}_\ell^T \mathbf{X}_\ell - \frac{w}{1 + w \delta} \mathbf{X}_\ell^T \left(\delta \left(\mathbf{I}_n - \frac{g_0}{g_0 + 1} \mathbf{H}_0 \right) + w \mathbf{H}_\ell \right)^{-1} \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y} \\ &= \mathbf{y}^T \mathbf{y} - \frac{w \delta}{1 + w \delta} \mathbf{y}^T \mathbf{X}_\ell \left(\mathbf{X}_\ell^T \mathbf{X}_\ell - \frac{w}{(1 + w \delta) \delta} \mathbf{X}_\ell^T \left(\mathbf{I}_n - \frac{g_0}{g_0 + 1} \mathbf{H}_0 + \frac{w}{\delta} \mathbf{H}_\ell \right)^{-1} \mathbf{X}_\ell \right)^{-1} \mathbf{X}_\ell^T \mathbf{y}, \end{aligned} \quad (\text{B.1})$$

where $\mathbf{H}_\ell = \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T$ and $\mathbf{H}_0 = \mathbf{X}_0 (\mathbf{X}_0^T \mathbf{X}_0)^{-1} \mathbf{X}_0^T = \mathbf{1}_n (\mathbf{1}_n^T \mathbf{1}_n)^{-1} \mathbf{1}_n^T = n^{-1} \mathbf{1}_n \mathbf{1}_n^T$. For the derivation of the first expression, see Woodburys matrix identity (Harville, 1997, p. 423–426). For large values of δ and $g_0 \gg \delta$ we have approximately $w \approx 1$, $\frac{w \delta}{1 + w \delta} \approx 1$ and $\frac{w}{(1 + w \delta) \delta} \approx 0$, which yields the approximation

$$\mathbf{y}^T (\mathbf{I}_n + \mathbf{X}_\ell \mathbf{V}_\ell^{(\text{CR})} \mathbf{X}_\ell^T)^{-1} \mathbf{y} \approx \mathbf{y}^T \mathbf{y} - \mathbf{y}^T \mathbf{X}_\ell (\mathbf{X}_\ell^T \mathbf{X}_\ell)^{-1} \mathbf{X}_\ell^T \mathbf{y} \equiv \text{RSS}_\ell. \quad (\text{B.2})$$

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